PROJECT ADMINISTRATION DATA SHEET

[X] ORIGINAL [ ] REVISION NO. ____

Project No. E-19-651 (R6027-0A0) GTRC/~~GTX~~ DATE 11 / 11 / 85

Project Director: M. G. White School/~~Lab~~ ChE

Sponsor: National Science Foundation

Type Agreement: Grant No. ECS - 8515177

Award Period: From 10/1/85 To 9/30/86 (Performance) 12/31/86 (Reports)

Sponsor Amount:	This Change	Total to Date
Estimated:	$	$ -0-
Funded:	$	$ -0-

Cost Sharing Amount: $ $1,500 Cost Sharing No: E-19-335

Title: Super Computer Use

ADMINISTRATIVE DATA OCA Contact John B. Schonk X 4820

1) Sponsor Technical Contact:

Frank Huband
National Science Foundation
ENG/ECS
Washington, DC 20550

(202) 357-9618

2) Sponsor Admin/Contractual Matters:

Joe Carrabino
National Science Foundation
DGC/ENG
Washington, DC 20550

(202) 357-9602

Defense Priority Rating: N/A Military Security Classification: N/A

(or) Company/Industrial Proprietary: N/A

RESTRICTIONS

See Attached N/A Supplemental Information Sheet for Additional Requirements.

Travel: Foreign travel must have prior approval – Contact OCA in each case. Domestic travel requires sponsor approval where total will exceed greater of $500 or 125% of approved proposal budget category.

Equipment: Title vests with N/A

COMMENTS:

This project is for Super Computer Use - no sponsor funds will be extended on this account.

No cost-sharing is required on this project.

COPIES TO: SPONSOR'S I. D. NO. 02 407 000.85.117

Project Director
Research Administrative Network
Research Property Management
Accounting
Procurement/GTRI Supply Services
Research Security Services
Reports Coordinator (OCA)
Research Communications (2)
GTRC
Library
Project File
Other A. Jones

FORM OCA 65 285

GEORGIA INSTITUTE OF TECHNOLOGY OFFICE OF CONTRACT ADMINISTRATION

SR669

SPONSORED PROJECT TERMINATION/CLOSEOUT SHEET

Date 2/16/87

Project No. E-19-651 School ~~Lab~~ CHE

Includes Subproject No.(s) N/A

Project Director(s) M. G. White GTRI / ~~GIT~~

Sponsor National Science Foundation

Title Super Computer Use

Effective Completion Date: 9/30/86 (Performance) 12/31/86 (Reports)

Grant/Contract Closeout Actions Remaining:

- [X] None
- [ ] Final Invoice or Final Fiscal Report
- [ ] Closing Documents
- [ ] Final Report of Inventions
- [ ] Govt. Property Inventory & Related Certificate
- [ ] Classified Material Certificate
- [ ] Other _____

Continues Project No. _____ Continued by Project No. _____

COPIES TO:

Project Director
Research Administrative Network
Research Property Management
Accounting
Procurement/EES Supply Services
Research Security Services
~~Reports Coordinator (OCA)~~
~~Legal Services~~

Library
GTRI
~~Research Communications (2)~~
Project File
Other Ina Lashley
Angela Jones
Russ Embry

Form OCA 60:1028

E-19-651

NATIONAL SCIENCE FOUNDATION
Washington, D.C. 20550

FINAL PROJECT REPORT
NSF FORM 98A

PLEASE READ INSTRUCTIONS ON REVERSE BEFORE COMPLETING

PART I–PROJECT IDENTIFICATION INFORMATION

1. Institution and Address	2. NSF Program	3. NSF Award Number
Georgia Institute of Technology Atlanta, GA 30332-0100	Super Computer Initiation	ECS-8515177
	4. Award Period From 10/1/85 To 10/1/86	5. Cumulative Award Amount 25 hours Computer time

6. Project Title

Super Computer Initiation: Molecular Orbital Calculations on Model Catalysts

PART II–SUMMARY OF COMPLETED PROJECT *(FOR PUBLIC USE)*

The grant was a zero budget, computer access time on the Purdue University Supercomputer. Before any computing studies were executed at Purdue, we attempted the process of converting our scalar code into vector code using the facilities at the University of Georgia Computing Center. The supercomputer at UGA is very similar to the one at Purdue. The migration of code from our scalar source to the target vector computer code showed less than 10% of the program could be vectorized. The failure to convert the scalar source program could be attributed to a number of "if" statements placed within "do" loops of the source code. This syntax, characteristic of Fortran programming language in the 1960's, is not vectorized by the vector compilers available to us. With only 10% of the source code vectorized, we sought other sources of code to perform the Huckel molecular orbital calculations.

Dr. E. Clementi of IBM's research center in New York was contacted. He is an expert in quantum mechanical calculations and is aware of the many different types of quantum mechanical programs. He suggested that we migrate our Huckel code on the IBM facilities. However, this effort would be unproductive since the resulting target code would run only on parallel processing machines. The Purdue machine is not a parallel processing machine; it is vector processing only. We could not obtain a source code for quantum mechanical calculations, suitable for the Purdue machine. Thus, we terminated any further attempts to use the computer funds provided by the grant.

PART III–TECHNICAL INFORMATION *(FOR PROGRAM MANAGEMENT USES)*

1. ITEM *(Check appropriate blocks)*	NONE	ATTACHED	PREVIOUSLY FURNISHED	TO BE FURNISHED SEPARATELY TO PROGRAM	
				Check (√)	Approx. Date
a. Abstracts of Theses	✓				
b. Publication Citations	✓				
c. Data on Scientific Collaborators	✓				
d. Information on Inventions	✓				
e. Technical Description of Project and Results					
f. Other *(specify)*					

2. Principal Investigator/Project Director Name *(Typed)*	3. Principal Investigator/Project Director Signature	4. Date
Mark G. White		1/23/87

NSF Form 98A (3-83) Supersedes All Previous Editions

Form Approved OMB No. 3145-0058

Final Report

National Science Foundation Grant

for

Supercomputing Time

Georgia Tech Account Number: E - 19 - 651

The grant was a zero-budget, computer access time on the Purdue University Supercomputer. Before any computing studies were executed at Purdue, we attempted the process of converting our scalar code into vector code using the facilities at the University of Georgia Computing Center. The supercomputer at UGA is very similar to the one at Purdue. The migration of code from our scalar source to the target vector computer code showed less than 10% of the program could be vectorized. The failure to convert the scalar source program could be attributed to a number of "if" statements placed within "do" loops of the source code. This syntax, characteristic of Fortran programming language in the 1960's, is not vectorized by the vector compilers available to us. With only 10% of the source code vectorized, we sought other sources of code to perform the Huckel molecular orbital calculations.

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